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Abstract

Uncertainties are inherent in computational fluid dynamics (CFD). These uncertainties need to be systematically addressed and managed. Sources of these uncertainties are identified and some aspects of uncertainty analysis are discussed. Some recommendations are made for quantification of CFD uncertainties. A practical method of uncertainty analysis is based on sensitivity analysis. When CFD is used to design fluid dynamic systems, sensitivity-uncertainty analysis is essential. The reliability and applicability of computer codes is established by a process called code certification.

Introduction

The commonly used word *"uncertainty" means lack of sureness or reliability about someone or something.* This word also means an error, but it does not mean a mistake. In a number of endeavors, the value of uncertainty is determined and decisions are made based on this value. The following are some examples of these endeavors: nuclear reactor analysis [1], structural engineering [2], experimental measurements [3], psychology [4] and artificial intelligence [5]. Uncertainties in risk assessment and management are of concern to people in various fields [6] such as decision analysts, aircraft designers, safety engineers, epidemiologists, toxicologists, chemists, biologists, economists, political scientist, sociologists, and lawyers. The significance of uncertainty in experimental measurements is illustrated by the requirement of the *Journal of Fluids Engineering* that "all papers considered for publication in this journal must contain an adequate statement of the uncertainty of experimental data." This journal also provides guidelines for estimating and presenting uncertainty. Thus, experimental data are considered seriously only if uncertainties are quantified. But computational results are considered for archival publications without quantification of uncertainties.

Recently, attempts [7]-[9] have been made to address numerical uncertainty. But CFD uncertainties need to be addressed. (The nomenclature of CFD is used to encompass a range of related areas such as computational aerodynamics, combustion, rarefied gas dynamics, and computational aerothermodynamics.) Often, the computational fluid dynamicists are concerned only about computation rather than about computation and fluid dynamics, abdicating responsibility for the latter to the experimenters. There are no standards for estimating and presenting CFD uncertainties. These uncertainties should be systematically addressed and properly managed. The objective of this paper is to identify uncertainties in CFD, discuss some aspects of uncertainty analysis, and to make some recommendations to quantify these uncertainties, using examples taken from computation of hypersonic flight estimates. The essence of these discussions is applicable to all speed regimes.

After a period of what was essentially hibernation, hypersonic research and technology development are presently being vigorously pursued. The United States [10], United Kingdom [11], West Germany [12], France [13], Japan [14], and the U.S.S.R. [15] have substantial programs. Among all these activities, the US effort related to the National Aero-Space Plane (NASP) Program is the greatest challenge and involves the largest commitment. This program has the potential of being a significant research and technology development program comparable in magnitude to programs such as the Manhattan Project, the Naval Reactors Program, and the Apollo/Saturn Program. Just as each one of these programs has made a major impact on science and technology conducted in the US [16] and on the nation as a whole, the NASP Program can make a major impact. (See also references [10] and [17]). For example, the NASP derived vehicles are likely to provide an access to space at a cost substantially lower than that for the space shuttle.

There are parallels between the design of space planes and that of nuclear systems, weapons, and reactors. First, a limited set of tests for gathering design data is possible. The design of both of these depends heavily on computer codes. Only after the first prototype is designed, built, and tested can a great deal of confidence can be developed for future such designs. In the field of reactor analysis, because of the responsibility placed on computer codes, a systematic effort was made to develop a practical uncertainty analysis method beginning in the early 1970s [18]. A frequently used method of conducting uncertainty analysis is based on sensitivity analysis. Once the uncertainty is determined, it is possible to design with a margin built in to reduce the risk associated with this uncertainty. Likewise, it is recommended that a systematic effort is required in CFD, particularly for design application which is the ultimate utility of CFD.

Significance of CFD in the Design of Space Planes

Subsonic, transonic, and supersonic aircraft are largely designed with data obtained from the ground-based test facilities. Very little CFD was used on currently operational aircraft built in the US. Beginning with substantial use of CFD in the design of Airbus A-310 [19] that reduced the overall wing design timescale by 35% compared to that of A-300, CFD is increasingly being used in the aircraft design process. Future aircraft are being designed with more CFD data and less test data than those data developed for the current aircraft. This trend is occurring because CFD helps to reduce the timescale for aircraft development and it is an appropriate tool for design optimization.

The NASP Program is a national effort to develop and demonstrate hypersonic technologies with the ultimate goal of single-stage-to-orbit (SSTO). This plane is a transatmospheric vehicle (TAV) with an air-breathing propulsion, horizontal take-off and landing, and long range hypersonic cruise in the atmosphere. This plane, designated as the X-30 aircraft (Fig. 1), is going to be largely designed by CFD, because of aeropropulsion issues that cannot be

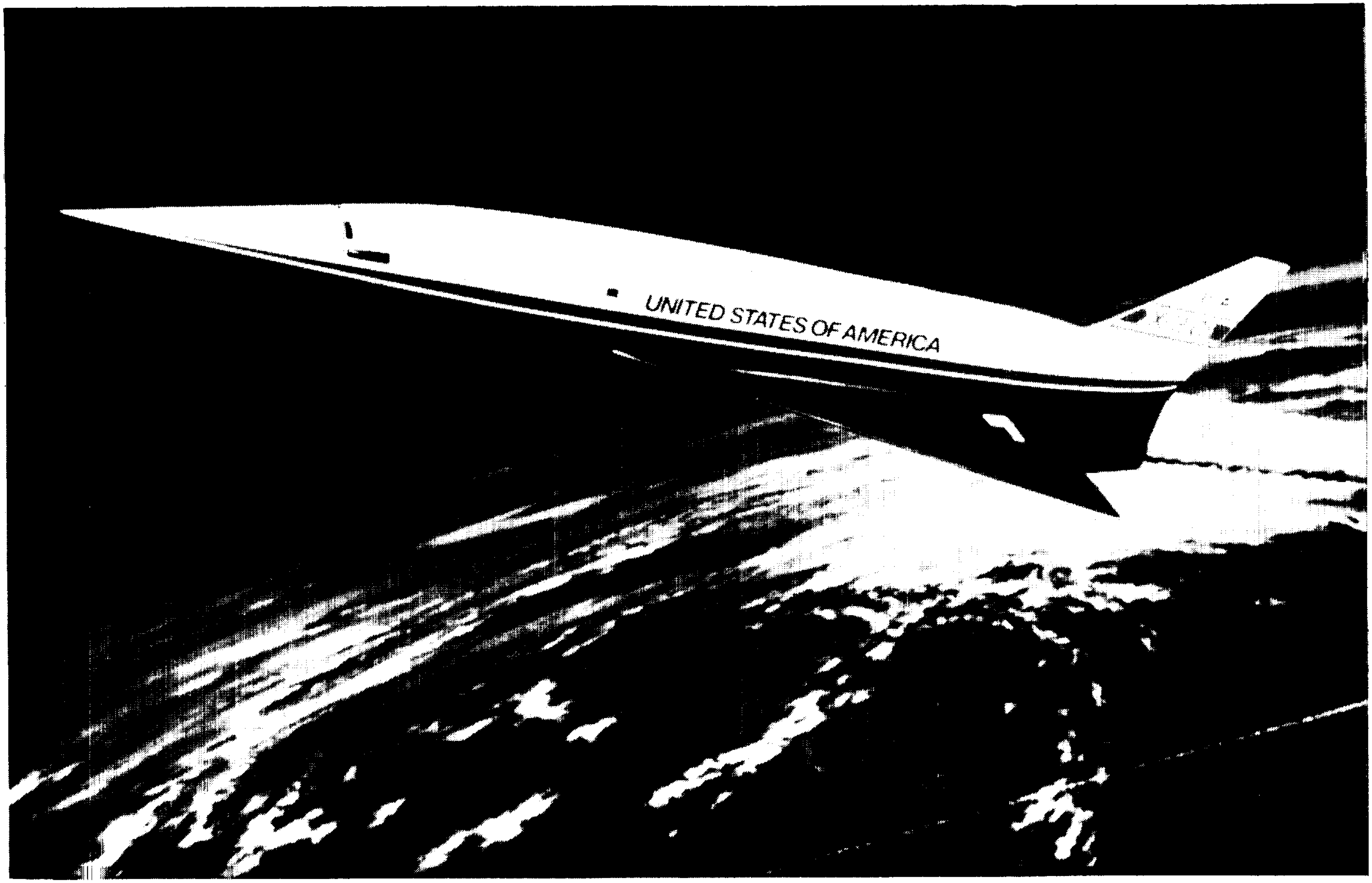

Fig. 1 The government baseline concept of the X-30 space plane.

duplicated in ground-based facilities (see, for example, Mehta [20]). Obviously, this places a great responsibility on computational fluid dynamicists to predict the performance quantities to a level of accuracy required for design purposes. They are also challenged to understand and quantify limitations of these predictions.

The importance of the aforementioned responsibility and challenge can be explained as follows. The traditional method of designing aircraft based on the ground-based test data is not appropriate for the design of space planes for the following reasons. First, there are fundamental difficulties in creating complete simulations in ground-based facilities. (See the discussions about these difficulties regarding existing and to-be-refurbished facilities in references [21-23]). Second, details of the upper atmosphere such as local composition, temperature, and turbulence are not known sufficiently to properly establish the relationship between flight conditions and ground-based data [22]. There are effectively two alternatives. The development of the aerospace plane may be postponed for as long as 10 years while a substantially large data base is developed using new test facilities in addition to those currently planned to provide data within next two or three years, and CFD is used to a limited extent. Alternatively, CFD is heavily used at Mach numbers above 10, along with measurements from available facilities (existing, refurbished, and new), to design this plane with sufficient margin for safety. The latter alternative is being pursued for the NASP Program [10]. Primarily, this decision is explained as follows: (i) The X-30 aircraft is a research and technology development aircraft. One of the technologies to be developed is the CFD design technology for hypervelocity vehicles. Substantial progress has been made in developing this technology since 1986 when the NASP Program formally began. Once this technology is developed, it can be used for designing NASP derivative space planes. (ii) Flight test data are essential for hypervelocity vehicle development. Aeropropulsion data associated with the complete aircraft are essential. Flight tests of the airframe or the engine alone have limited utility in the design process.

Uncertainties in Computational Fluid Dynamics

The phrase *computational fluid dynamics* encompasses two different disciplines, computation and fluid dynamics. Together these disciplines are used for numerical simulation of physical and chemical reality through modeling. This numerical simulation is acceptable if it accurately reproduces the reality. Frequently, this cannot be achieved because both fluid dynamics and computation contain uncertainties that affect the computed estimates. The reason for this situation is obvious. The numerical simulation attempts to describe natural reality. A simulation is not reality. In addition to this scientific uncertainty in CFD efforts, there is a human factor uncertainty. These uncertainties are summarized in Fig. 2, and they are discussed below.

Fluid Dynamic Uncertainties

There are three sources of uncertainties related to physics and chemistry. First, the uncertainty is caused by isolation of (physical and/or chemical) phenomena, either deliberate or unavoidable. In order to understand certain phenomena, it is customary to set up a unit (that is, a benchmark or building-block) problem demonstrating these phenomena, assuming

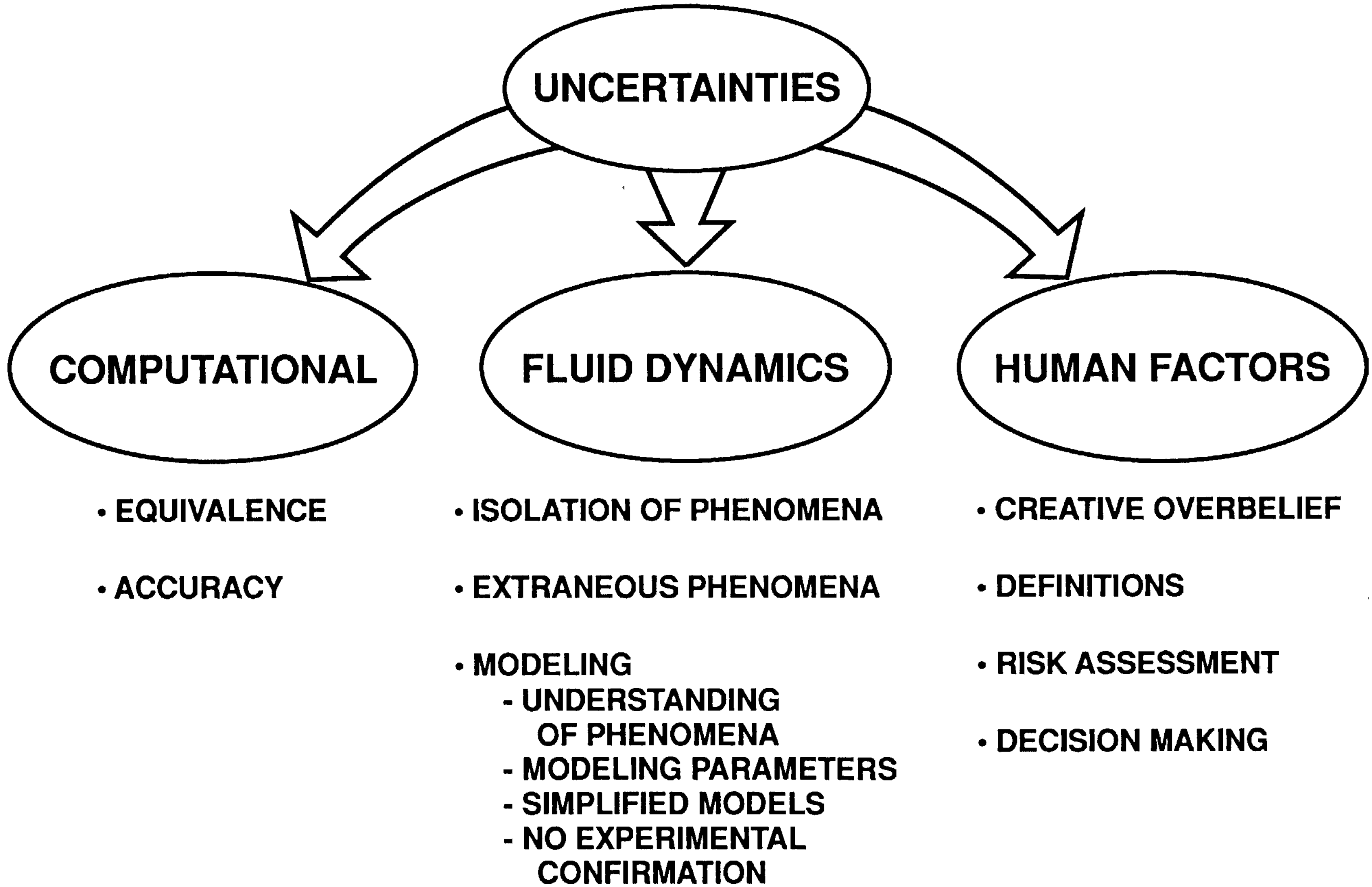

Fig. 2 Uncertainties in computational fluid dynamic results.

that there is either absolutely no influence or perfectly known influence on these phenomena of other natural phenomena. Sometimes lack of knowledge leads to isolation of phenomena. On the other hand, unavoidable isolation of phenomena takes place when it is not possible to address all relevant phenomena simultaneously. In either case, an approximation or an uncertainty is introduced. Second, the uncertainty is caused by the insertion of extraneous phenomena. When the reality of interest either cannot be simulated or is difficult to simulate, sometimes an alteration other than a simplification (isolation) of this reality is made so that this modified reality can be simulated. This introduction of extraneous phenomena may perturb the manifestation of existing phenomena. Third, the uncertainty is caused by improper modeling of the phenomena under consideration. A model describes reality in mathematical and/or empirical terms. The uncertainty is related to the validity of the model. Specifically, the sources of modeling uncertainty are the following: (i) The phenomenon under investigation is not thoroughly understood. (ii) Parameters used in the model are known with some degree of uncertainty. (iii) Appropriate models are simplified introducing uncertainty. (iv) An experimental confirmation of the model is not possible or not available.

In the design of the space plane, "aeropropulsion dynamics" is the most significant discipline. It includes aerodynamics, aerothermodynamics, propulsion, and aerodynamic-propulsive integration. Five phenomena are critical in aeropropulsion dynamics at hypervelocities: boundary layer characteristics, shock wave/boundary layer interaction, mixing of fuel and air, chemical kinetics, and low density effects at intermediate (say from 40 km to 80 km) and high (above 80 km) altitudes. Each of these phenomena may be further fragmented or isolated by imposing some constraints on them. The following are some examples: (i) The boundary layer transition from a laminar to turbulent flow is considered to depend on Mach number, Reynolds number, and the wall temperature without considering chemical kinetics. (ii) Different types of shock wave/boundary layer interaction phenomena are identified as incident shock interaction, compression corner interaction, corner flow interaction, glancing interaction, shock train interaction, shock/shock interaction, and shock/cooling layer interaction. Some of these interactions may occur side by side, which may cause them to influence each other. (iii) The effect of combustion instability on the mixing process is not considered. (iv) In chemical kinetics, an idealization is based on which initiation, branching, and termination reactions are considered between H_2 and O_2. (v) The low-density effects in the nose region and leading-edge region are neglected when the rest of the flow can be handled by the continuum, no-slip assumption.

A consequence of the isolation of phenomena illustrated in example (v) is explained as follows. There may be a mixed flow, continuum transitional flow around the nose region and continuum flow downstream of this region. The shock structure and chemical kinetics taking place in this region would have an impact on transition location, the length of the transition region, and the characteristic of the flow entering the engine.

Isolation of phenomena may also occur under the following condition: Design problems involve more phenomena than those considered in unit problems. Modeling of phenomena associated with unit problems and those associated with design problems may differ. The overall effect of the interaction of phenomena associated with different unit problems is unlikely to be simply additive.

Since the ground-based facilities cannot fully simulate hypervelocity flight conditions, they may produce phenomena other than those of interest. An example of extraneous phenomena uncertainty is the simulation of ground-based combustor flow with chemical reactions in addition to those expected under flight conditions.

There are various sources of uncertainty of modeling: the basic flow equations, transition model, transition length model, relaminarization model, turbulence model (momentum and heat fluxes), relationship between viscous stress and strain rate, relationship between the first and second coefficient of viscosity, chemical reaction rates, vibrational and radiation excitation rates, surface chemical reaction rates (surface catalysis), gas and transport properties, and upstream flow conditions. The modeling uncertainty includes the uncertainty of the range of validity of the model. The term "basic flow equations" considers basic models for continuum, continuum transitional, and rarefied flows, dimensionality, etc. Further, transition and turbulence modeling of both attached and free shear layers are considered.

Computational Uncertainties

Once the modeling equations (which include the initial and boundary conditions) are determined, numerical algorithms are developed to solve them and computer codes are constructed. There are two sources of uncertainties of computation: equivalence and numerical accuracy. Further, a computer code may contain mistakes.

The computational model need to describe the "reality" contained in the theoretical (mathematical and/or empirical) model. A departure from equivalence of the two realities introduces errors. At times, this departure is caused by the need for an efficient and robust numerical algorithm. Examples of this departure are the following: (i) The fitting of strong shock waves, such as the bow shock wave at intermediate and high altitudes, would not resolve the shock structure, thereby altering the flow around the nose and the flow downstream of it. (ii) Numerical algorithms for complex problems generally use the one-dimensional Riemann solver without taking into account multi-dimensional wave propagation. Under certain conditions, these algorithms may produce a contact discontinuity instead of a shock wave, and vice versa. (iii) The computational model may produce an asymptotic (steady-state, periodic, or chaotic), global solution that is a spurious solution of the theoretical model. Some numerical algorithms (time discretization schemes and/or nonlinear schemes for spatial discretization schemes) produce such solutions [24]. Nonequilibrium, hypervelocity flows are typically governed by reaction-convection-diffusion equations containing nonlinear source terms. These equations may exhibit a nonlinear dynamical behavior; for example, they may have well-separated multiple solutions. The discrete (computational) model should be able to determine the solution that corresponds to that of the differential (theoretical) model.

There are three sources of uncertainty related to numerical accuracy. First, an algorithm consists primarily of an approximation of the mathematical model owing to discretization. In the limit of the spatial and temporal grid sizes approaching zero, a consistent discretization would not have any discretization errors. In practice, this limit cannot be taken. For instance, algorithms for combustor flows may modify the combustion phenomena owing to numerical dissipation (diffusion). Further, the solution procedure for the inviscid part of the NS equations requires numerical damping (see for example [25] and [26]), thereby influencing viscous solutions. Second, a solution procedure used in an algorithm may contain an approximation. For example, the solution accuracy is dependent on the convergence criteria used in any iterative procedure. Third, techniques used for presentation of computed results is a source of uncertainty. An example is the presentation and interpretation of results using graphical techniques, which have inherent errors. (See also [27].)

A computer code can be a source of errors. The logic of the code involves the following: consistency of computer instructions with the numerical algorithm (model) and data management (internal and input/output). Coding errors are mistakes, not uncertainties. These mistakes can be eliminated by either checking the logic or by developing independently another code to confirm the results. (Computer hardware errors are not considered.)

Human Factor Uncertainties

There are four types of human factor uncertainties: phenomenon of creative overbelief [28], uncertainties about definitions, uncertainties about risk assessment, and uncertainties in decision making. The first two types can be eliminated with systematic questioning, whereas the latter two types of uncertainties are difficult to eliminate. These two principally arise when CFD is used in the design process.

Usually a person develops an emotional attachment to his creation which tends to visualize this creation as a reality based on insufficient evidence. The competitive market generally encourages overselling and fostering of creative overbelief. Uncertainties about definitions are caused by ambiguity concerning meaning and interpretation. Two examples are discussed below. Uncertainties about risk assessment arise from disagreements concerning what constitutes a risk and what is considered to be an acceptable risk. For example, what are acceptable risks due to fluid dynamic uncertainties and computational uncertainties within the flight envelope of the X-30 aircraft? Uncertainties in decision making arise because of insufficient information. For example, how does one determine some of the fluid dynamics and computational uncertainties without flight test data?

An Ad Hoc Committee on Code Validation of the Aeronautics Advisory Committee of NASA has defined CFD code calibration as follows [29]: "CFD Code Calibration: The comparison of CFD code results with experimental data for realistic geometries that are similar to the ones of design interest;" this comparison is "made in order to provide a measure of the code's capability to predict specific parameters that are of importance to the design objectives without necessarily verifying that all the features of the flow are correctly modeled." In this definition, the phrase "to provide a measure of the code's capability to predict" is ambiguous. A comparison between computed results and experimental data for a design-like geometry is not sufficient to justify declaring the code to be a calibrated code.

Referring to definitions of code validation and code calibration as worded by the above Committee, Marvin [30] states the following: "Such definitions refer mainly to the completeness of the process. For the purposes of this paper, validation will refer to the overall process with the understanding that completeness will be evidenced in the depth and scope of carrying out the process." This quote illustrates uncertainty caused by interpretation and that due to meaning. The definition of code validation by the Committee explicitly contains the phrase "validation can occur only when." This definition spells out the conditions under which a code can be considered to be a validated code. However, the above quote interprets code validation to be a process. When a claim is made that "code validation is done," what does one understand by it? The code may have undergone the process of validation or the code has achieved the status of being a validated code. Having two different meanings of "validation" introduces uncertainties. On the other hand, consider the second sentence of the above quote, which defines validation. In this definition, the following phrase is meaningless: "completeness will be evidenced in the depth and scope of carrying out the process." What is the status or credibility of a code, if completeness is not achieved? In addition to this ambiguity, "carrying out the process" does not necessary lead to a validated code.

Uncertainty Analysis

Generally, *uncertainty analysis is defined as the analysis of the effect of uncertainties involved in all stages of a process on the final responses.* This process, for example, may be an experimental process or a computational process with the responses being experimental data or computed results, respectively. There are two approaches to conducting the uncertainty analysis: experimental and computational. In CFD, the experimental approach is used more often than the computational approach. In nuclear reactor analysis, the computational approach is extensively used [18]. The other examples are air quality studies for protecting the environment (for example, [31]) and nuclear waste isolation studies (for example, [32] and [33]). Both approaches need to be fully and systematically exploited. They are equally essential for establishing the credibility of the hypersonic flight estimates, which in turn helps to establish the credibility of the design.

Experimental Approach

Since CFD numerically simulates physical and chemical reality through modeling, the obvious uncertainty analysis method consists of comparisons between computed results and measurements. This experimental approach has its own limitations, primarily the following: uncertainties, the capability for conducting relevant tests, and insufficiency of data.

Uncertainties are also inherent in experimental fluid dynamics. Both measurement and fluid dynamics contain uncertainties. The fluid dynamic uncertainties arise when ground-based testing is done to simulate flight reality. Two sources of uncertainties related to fluid dynamics are phenomena of isolation and extraneous phenomena. In case of measurements, ground-based or flight, there are interference uncertainties and data uncertainties. *Unless these measurement uncertainties are known, uncertainties of computed results cannot be determined with test data. (More importantly, the credibility of a design based on test data whose credibility is not established by indicating measurement uncertainties is questionable.)* Further, there are human factor uncertainties, in particular those related to creative over-belief and definitions. An example of the former is the attitude that measurements are the reality. An example of the latter is the false assignment of significance to what has been measured. (Uncertainties due to risk assessment and decision making need to be considered, if test data are to be used for design purposes.)

The fluid dynamic uncertainties are illustrated as follows. The chemical phenomena associated with air are not addressed when ground-based aerodynamic tests are conducted in a nitrogen wind tunnel at high hypersonic Mach numbers. Sometimes the heat transfer boundary condition in ground-based facilities are different from those observed in flight. In some instances, the ground-based facilities introduce phenomena that are not likely to occur in flight. For example, alterations may be caused in the flow owing to effects of additional chemical species, unsteadiness, and disturbances during propulsion tests. In most of the existing ground-based facilities, flow conditions upstream of the test section (freestream conditions) are not sufficiently well known [22]. These conditions may introduce extraneous phenomena. *Without knowing the freestream conditions, meaningful computations cannot be done for comparison with test data.* Under such circumstances, the CFD that "confirm" the ground-based tests may be uncertain for estimating flight quantities. Another source of uncertainty is the process of extrapolating from ground-based test conditions to flight conditions. The result of an extrapolation involving a change in fluid dynamics is more uncertain than that of an interpolation without any such change.

There is interference or interaction between the test device and the flow of interest. The manner in which measurements are taken influences the measured quantities, introducing interference uncertainties. It is impossible to completely correct for these interferences. Ronen [18] justifies this statement using the uncertainty principle (Heisenburg) and the complementarity principle (Bohr). There are two types of interference uncertainties associated with the measuring system, system-sensor interaction uncertainties and system disturbance uncertainties.

Data uncertainties are the residual errors after all corrections have been made to the measured quantities. The uncertainty in a measurement is generally defined as the difference between measured value and the true value of the quantity being measured. There are three types of uncertainties: fixed, random, and variable but deterministic [34]. These uncertainties are also categorized as bias (fixed) and precision (random and variable but deterministic) uncertainties. A standard measurement uncertainty methodology has been adopted by a number of organizations such as SAE, ASME, AIAA, and JANNAF. Discussions of measurement uncertainty analysis may be found in several references, such as: Coleman [3], Moffat [34], ANSI/ASME Standards on Uncertainty [35], and Thompson, Kimzey, and Boals [36].

If the levels of measurement uncertainties are acceptable and there is an acceptable level of agreement between the computed results and measurements, then the computer code providing these results is credible. This means that both the fluid dynamics model and numerics are satisfactory. If the level of agreement is not acceptable, then the code may still be acceptable. A possible source of this unacceptable level of agreement is the manner in which the code is being used. Alternatively, fluid dynamics and/or numerics is unsatisfactory and/or the numerical algorithm (model) may not be programmed properly. What are considered as "acceptable" computed results is determined by the numerical accuracy requirements for these results. These are set by the utility of these results. When the experimental approach is used, the uncertainties in the computed results are the differences between measurements and computed results. This definition assumes that the computed results are accurate.

The experimental approach by itself is of limited utility for flight estimates because of the following reasons: (i) There is insufficiency of data, ground-based or flight. It is not always possible to measure all quantities of interest, those necessary, and as often as required for a proper uncertainty analysis. (ii) Often the relevant hypervelocity tests are not possible to carry out. Further, ground-based facilities may introduce fluid dynamic uncertainties, as illustrated above. (iii) This approach does not account for uncertainties in computation, that is, the accuracy of the computed results without a consideration of the experimental data. These uncertainties need to be identified when computed results are compared with measurements. Almost invariably, an excellent comparison between computed results and measurements is used to justify the validity of the computational model, without demonstrating, for example, the effect of grid refinement on the computed result. (iv) The experimental approach provides some, but not a sufficient, guidance for obtaining computed results with the same uncertainties or accuracy at conditions other than those considered, but with the same fluid dynamics.

Computational Approach

The second approach to conducting the computational fluid dynamic uncertainty analysis is the computational approach. This approach essentially does not utilize test measurements. In this case, uncertainties in modeling, uncertainties caused by input parameters, uncertainties in equivalence, and uncertainties in numerical accuracy are determined separately. Modeling uncertainties are generally conducted by those concerned with fluid dynamics. Input uncertainties are usually investigated by those interested in design and safety. Equivalence uncertainties and accuracy uncertainties are mainly of concern to people who are developing algorithms. However, all of these uncertainties are important. For example, the determination of modeling uncertainties is inconclusive without accuracy uncertainties. The theoretical model, the computational model, and the input parameters fix the accuracy that can be obtained.

When a test confirmation is not possible or available, it is sometimes possible to obtain an estimate of the uncertainty by computing the result in question with different models. For example, the intermediate and high altitude shock-on-shock heating on a cowl lip may be investigated by the Navier-Stokes (NS) equations, continuum equations more advanced than the NS equations, and the Boltzmann equation. The sensitivity of different transition models on heat transfer and skin friction and consequently on the take-off gross weight (TOGW) of the space plane can be studied to determine the uncertainty due to transition model. Similarly, uncertainties of turbulence models may be studied by considering models of increasing complexity. Although comparative studies involving different turbulence models are being done from the point of view of fluid dynamics in unit problems, they need to be done also for design-like problems and for determining the uncertainties in the design, for example in the TOGW.

Sometimes a simplified model is used although an accurate model is available. For example, the parabolized NS equations may be used rather than full NS equations. Another example is the use of a smaller set of finite rate (chemical) reactions than those considered necessary. There are two ways of estimating uncertainties resulting from the use of a simplified model. The obvious procedure for obtaining the uncertainties is to compute using both the simplified and complex model and determine the difference between the two sets of results. Another way is to determine, if feasible, the perturbation operator, which is the difference between the complex model operator and the simplified model operator. Then it may be possible to obtain the uncertainty based on the perturbation theory [37] or functional analysis [18].

A practical uncertainty analysis method for determining the uncertainties of the input parameters is based on sensitivity analysis. These parameters include the computational model parameters and specifications, for example, grid spacing, turbulence model constants, the order of numerical scheme, and initial and boundary conditions. *A sensitivity is a measure of the influence of a given input parameter on the computed results*, primarily performance estimates in design applications. Generally, *sensitivity analysis is defined as the procedure to determine sensitivities of input parameters on output results.* This analysis provides guidance with respect to the identification of the important contributors to uncertainty, helps to assess confidence levels in computed results, and assists in further development of the computational model. This analysis is particularly useful when large computer codes are used for modeling complex phenomena. It is being used, for instance, in problems exhibiting phenomena associated with heat and mass transfer, chemical kinetics, and nuclear reactor physics. Further, sensitivity analysis can be used in selecting solution-adaptive space and time steps (see for example, [38]).

Sensitivity analysis is crucial for establishing the credibility of a design and for design optimization. Assume that the computational model is appropriate. The acceptability of computed performance estimates is determined by the sensitivities of specifications to these estimates for the system under consideration. The requirements of acceptable accuracy for these estimates are set by their sensitivities to uncertainties in computed estimates. Some examples of sensitivities of space plane designs to performance estimates are discussed by Gregory [39], Mehta [20], and Gregory [40]. It is relatively convenient to conduct sensitivity analysis and design optimization with computers, but rather difficult to do so with test facilities, ground-based or flight.

Different methods are available for conducting sensitivity analysis: the brute force method, statistical methods, and deterministic methods. In the brute force method with N input parameters, a linear sensitivity and a nonlinear sensitivity, respectively, require $N + 1$ and $2N^2 + 2N + 1$ different computer solutions in order to determine sensitivities of one computed result. The other two methods greatly reduce the number of solutions needed. The response surface method, the Monte Carlo method and the Fourier Amplitude Sensitivity Test are examples of statistical methods. The adjoint method is an example of a deterministic method. Once the sensitivities are determined the uncertainty analysis is carried out to obtain uncertainties. Further, it is possible to obtain uncertainties in a new system, close to that in which uncertainties are known, without conducting the uncertainty analysis for this new system. The theoretical basis for the various sensitivity analysis methods and the uncertainty analysis is given in the book entitled *Uncertainty Analysis* and edited by Ronen [18]. The application of these sensitivity-uncertainty analysis methods to computational fluid dynamics is a new research activity, particularly in aeropropulsion dynamics.

Two major concerns of people who are developing numerical algorithms are the equivalence between theoretical and computational models and about computational accuracy. Uncertainties due to a lack of this equivalence and those due to a lack of numerical accuracy are rarely quantified for equations other than model equations used in the development of numerical methods. The only way the former uncertainties can be determined is by comparing two computed results, one with equivalence and one without equivalence. The latter uncertainties related to discretization is done by computing grid-independent results. A grid sensitivity analysis provides the sensitivity of the computed results to the grid size. But the Taylor series analysis for obtaining the leading truncation terms due to discretization does not quantify uncertainties. Algorithms to solve ordinary differential equations usually contain relative error estimates. These algorithms are not of concern here.

Reliability of Computer Codes

The lack of knowledge about the degree of credibility (confidence level) of results generated by a computer code introduces uncertainties and that about proper usage of this code creates mistakes. These uncertainties are not treated separately as they are related to the CFD uncertainties discussed previously. The credibility is established by addressing the computational fluid dynamics uncertainties and quantifying them. This process of establishing credibility also determines reliability and limits of applicability of the code.

Although an Ad Hoc Committee on Code Validation of the Aeronautics Advisory Committee of NASA has defined "CFD code validation" and "CFD code calibration" [29], these definitions are not useful or practical [20]. Definitions by themselves are not enough. There has to be an agreed-upon comprehensive and systematic process to establish the reliability and limits of applicability of the code. This process is called "code certification" [41], and it is defined as follows [20]: "The process of evaluating a computer code in terms of its logic, numerics, physics/chemistry, and the results, to ensure compliance with specific requirements." These requirements depend on the utility of computed results. These requirements may change, but the process is the same. They are determined by computational fluid dynamicists, designers or users, and experimenters.

The development of a standard was suggested [20] to guide the process of CFD code certification that would ensure and improve the credibility of the computed results and consequently that of the corresponding computer code. There is a precedent for this suggestion. The nuclear industry has a standard for guiding the "verification and validation" of scientific and engineering computer programs [42]. Agee and Hughes [43] have presented a report discussing experiences with this standard.

The CFD design technology development for space planes will be done by satisfying the "method-confident code" [20] requirements of code certification, in the absence of flight data. These requirements are the following: "A certification by computer simulations is achieved if the following conditions are satisfied: (a) A systematic determination of numerical accuracy of performance quantities is carried out. (b) The computed physics/chemistry is qualitatively satisfactory. (c) A part of physics/chemistry modeled in the code has been verified by (ground-based and flight) experiments, limited to this physics/chemistry. The range of applicability of the method-confident code is fixed by the similarity of physics/chemistry and body shapes." Confidence is gained in a code by satisfying requirements of numerical accuracy based on design sensitivities and a circumstantial evidence concerning the appropriateness of the fluid dynamics that is modeled in the code. When the appropriate flight data are available, the circumstantial evidence is replaced with actual evidence.

Concluding Remarks

A consideration of numerical uncertainties only partially addresses computational fluid dynamic uncertainties. These uncertainties are related to both computation and fluid dynamics parts of computational fluid dynamics. These are introduced by a lack of equivalence of theoretical and computational models, unsatisfactory computational accuracy, isolation of phenomena, extraneous phenomena, improper modeling of phenomena, and by human factors. These uncertainties need to be addressed systematically and properly managed. There are two approaches of uncertainty analysis, experimental and computational. Both of these are equally important. In the computational approach, the use of sensitivity-uncertainty analysis is suggested. Although these aspects of uncertainty in computational fluid dynamics are discussed with examples taken from hypervelocity aeropropulsion dynamics problems of space planes, the essence of this discussion is applicable to other speed regimes and to other fluid dynamic systems.

The ultimate utility of CFD is in the design of fluid dynamic systems. CFD may be used in the design process directly or indirectly. In the latter case, the engineering or simplified CFD design methods and/or values are improved or calibrated utilizing complex CFD methods and/or values. The credibility of CFD codes is established by code certification, which is a process for eliminating mistakes in codes and for determining their reliability and applicability.

The design of space planes renews an old problem, hypersonic transition, and introduces new problems, compressible turbulence modeling and supersonic combustion. In order to address these problems in a practical manner, programmatic research [20] is required. This puts the emphasis on sensitivities and uncertainties. Further, the sensitivity-uncertainty analysis helps to define a safe margin to account for uncertainties.

Specifically, the following recommendations are made to reduce uncertainties in computed hypersonic flight estimates:

- Uncertainties in measurements and computations must be quantified for establishing their credibility.
- Freestream conditions associated with tests, ground-based or flight, must be known.
- Sensitivity of computed performance estimates to CFD uncertainties need to be quantified.
- Sensitivity-uncertainty analysis is essential for developing credibility of any design.

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16. Abstract

Uncertainties are inherent in computational fluid dynamics (CFD). These uncertainties need to be systematically addressed and managed. Sources of these uncertainties are identified and some aspects of uncertainty analysis are discussed. Some recommendations are made for quantification of CFD uncertainties. A practical method of uncertainty analysis is based on sensitivity analysis. When CFD is used to design fluid dynamic systems, sensitivity-uncertainty analysis is essential. The reliability and applicability of computer codes is established by a process called code certification.

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